Pentane

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 39.4 °C

Global applicability domain: Inside

Local applicability domain index: 7.88e-01

Confidence level: 5.07e-01

Nearest Neighbors from the Training Set

Image not found
Pentane
Measured: 36.0
Predicted: 39.4

Image not found
2-Methylbutane
Measured: 27.8
Predicted: 35.4

Image not found
Propane, 2,2-dimethyl-
Measured: 9.50
Predicted: 30.1

Image not found
t-Butylchloride
Measured: 50.5
Predicted: 58.0

Image not found
(2H9)-tert-Butyl chloride
Measured: 50.5
Predicted: 58.0

Image not found
Diethylboron
Measured: 112
Predicted: 70.5